X-ray Diffraction Study of Fe_xO at High Pressure and Temperature: Magnetite Exsolution and Thermal Expansion *	X17B1

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Effect of defect concentration on the thermal expansion of wustite has not been well studied. Overall, only very few attempts have been made regarding this issue at atmospheric pressure. In general, such a volume-related property in wustite is more difficult to study than in most defect-free materials, because the arrangement of defect clusters and the extent of magnetite exsolution may adjust to changes in temperature Nevertheless, thermal expansion of wustite from available experimental determination (Hayakawa, 1972) does not appear to vary with stoichiometry. This measurement, however, was limited to the temperature range 1223-1323 K and to the composition range x = 0.88 - 0.95, thus unable to provide reliable account of the effect of defect concentration on the thermal expansion.

In this work, the isobaric volume-temperature measurements from synchrotron x-ray diffraction experiments were carried out at pressures of 1.9, 2.6, and 5.4 GPa with $Fe_{0.945}O$ as the starting material. The results reveal that the composition change of wustite and hence rearrangements of defect structures are primarily attributed to the exsolution of magnetite at temperatures of 523-723 K. In the ranges of 300-673 K and 773-1073 K, the contribution of compositional variations to the volumes changes of wstite is small, within uncertainty of the experiments and in agreement with previous findings. The observed volume changes or thermal expansion of this study can thus be attributed to the metal-oxygen bond expansion. Because of magnetite exsolution, two volume-temperature curves are determined in each experiment 1.9, 2.6, and 5.4 GPa, with a break at the temperatures between 673 and 773 K. These experiments are thus capable of yielding thermal expansion data for wustite of two different compositions, $Fe_{0.99}O$ and $Fe_{0.945}O$. At all three pressures, $e_{0.945}O$ shows a slope of $(\partial V/\partial T)_P$ that is about 30% larger than $Fe_{0.99}O$, providing the first experimental evidence of a substantial difference in thermal expansitivity between iron-rich and more iron-deficient wustite. Thermal expansion coefficients of $Fe_{0.99}O$ and $Fe_{0.945}O$, decrease, as expected, with increasing pressure. At 8.2 GPa, no magnetite exsolution was observed, and a smooth volume-temperature curved is obtained for Fe_xO with $x \approx 0.95$, with a thermal expansion coefficient that is consistent with the low pressure data.

Reference:

Hayakawa, M., Cohen, J.B. and Reed, T.B., J. Am. Ceram. Soc. 55: 160-164, 1972

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